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% Male Rat Liver In Vitro MCMC simulation file
% Three chains can be run by selecting different seernd
% and changing the output file name

prepare @clear
prepare @all

VVIALF=0.01165; %% Male ==VVIAL=.0119573;
VVIALM=0.0119573;
VMED=.001;
VINJF=0.0002; %% Male ==VIN=0.0003858 !important
VINM=0.0003858 ;
VAIRF=VVIALF-VMED;
VAIRM=VVIALM-VMED;
TSTOP=1.2;
TF=0.;
TI=0.2;
PROT = 1.0;
P1 = 0.69;
WESITG=0;
WEDITG =0;

CINT = 0.1 ;
MAXT = 0.001 ;
TSTOP = 1.1

KG1 = 0.45 ;

seedrnd(45526)
%seedrnd(334485)
%seedrnd(998754)

global _cal
global _time
global data
global tFindex
global tMindex

global CCC
global firstT
global lastT
global firstD
global lastD
global ControlData

use ControlData.m
use FemaleData.m
use MaleData.m

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dataF = [FratFLiver(:,IDf_270ppm : IDf_1ppm)];
dataM = [FratMLiver(:,IDm_264ppm : IDm_50ppm)];
data = NaN* ones([25, 8]); % corresspone to max 25 timepoints and 5 dose
each gender
data(1:6, 1:5) = dataF ;
data(1:25, 6:8) = dataM;
firstT = [1, 1]
lastT = [6, 25]
firstD = [1, 6]
lastD = [5, 8]
tFindex = FratFLiver(:, IDf_time);
tMindex = FratMLiver(:, IDm_time);

AA=dataF(1,:)*(VAIRF+P1*VMED);
BB=dataM(1,:)*(VAIRM+P1*VMED);
CCC = [AA, BB];
data = log(data);

function preds = getpreds(Vmax, Km, VK, A10, Gender)
    global _cal
    global _time
    global tFindex
    global tMindex
    global ControlData

    % draw back ground loss rate
    tmp = ceil(rand*500);
    lossR = ControlData(tmp);

    setmdl("VMAX1", exp(Vmax)); % reset model parameter as global
variables
    setmdl("KM1", exp(Km));
    setmdl("VK", VK);
    setmdl("A10", A10);
    setmdl("RLOSS", exp(lossR));

    if Gender==1
        tindex = tFindex;
        setmdl("VVIAL", 0.01165);
        setmdl("VINJ", 0.0002);
    else
        tindex = tMindex;
        setmdl("VVIAL", 0.0119573);
        setmdl("VINJ", 0.0003858);
    end

    data @clear
    data("SAMPTIMES", ["T"], tindex);

    start @nocallback

    preds = NaN*ones(length(tindex), 1);

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for i = 1:length(tindex)
    idx = find(_time == tindex(i));
    if(idx ~= [])
        preds(i) = max(0.0, _cal(idx));
    end
end

preds = log(preds);

use ".\MCMCscripts\mmminvitroliv1lvl.m"

chains = runmcmc();

save @file=mratliverredo1.dat @format=ascii @separator=tab chains
```